SM358/Specimen Equations booklet

Wave mechanics

$$\widehat{\mathrm{x}} \Longrightarrow x \qquad \widehat{\mathrm{p}}_x \Longrightarrow -\mathrm{i}\hbar\frac{\partial}{\partial x}$$

$$\mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = \widehat{\mathrm{H}}\Psi \qquad \mathrm{i}\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi}{\partial x^2} + V(x)\Psi(x,t)$$

$$\Psi_n(x,t) = \psi_n(x)\,\mathrm{e}^{-\mathrm{i}E_nt/\hbar} \qquad \Psi_{\mathrm{dB}}(x,t) = \mathrm{e}^{\mathrm{i}(kx-\omega t)} \quad p_x = \hbar k \quad E = \hbar\omega$$

$$\widehat{\mathrm{H}}\psi_n(x) = E_n\psi_n(x) \qquad -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi_n}{\mathrm{d}x^2} + V(x)\psi_n(x) = E_n\psi_n(x)$$

$$p_i = \left|\int_{-\infty}^{\infty}\psi_i^*(x)\,\Psi(x,t)\,\mathrm{d}x\right|^2 \qquad \text{probability density} = |\Psi(x,t)|^2$$

$$\langle A\rangle = \sum_i p_iA_i \qquad \langle A\rangle = \int_{-\infty}^{\infty}\Psi^*(x,t)\,\widehat{\mathrm{A}}\Psi(x,t)\,\mathrm{d}x$$

$$\Delta A = \left(\langle A^2\rangle - \langle A\rangle^2\right)^{1/2} \qquad \Delta x\,\Delta p_x \geq \hbar/2$$

$$\frac{\mathrm{d}\langle x\rangle}{\mathrm{d}t} = \frac{\langle p_x\rangle}{m} \qquad \frac{\mathrm{d}\langle p_x\rangle}{\mathrm{d}t} = -\left\langle\frac{\partial V}{\partial x}\right\rangle$$

$$E_n = \frac{n^2\pi^2\hbar^2}{2mL^2} \quad n = 1, 2, \ldots \qquad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)$$

$$\psi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi x}{L}\right) \quad (n \text{ odd}) \qquad \psi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) \quad (n \text{ even})$$

$$E_n = (n+\tfrac{1}{2})\hbar\omega_0 \quad n = 0, 1, \ldots \qquad \omega_0 = \sqrt{C/m} \qquad a = \sqrt{\hbar/m\omega_0}$$

$$\widehat{\mathrm{H}} = \left(\widehat{\mathrm{A}}^\dagger\,\widehat{\mathrm{A}} + \tfrac{1}{2}\right)\hbar\omega_0 \qquad \widehat{\mathrm{A}}\widehat{\mathrm{A}}^\dagger - \widehat{\mathrm{A}}^\dagger\widehat{\mathrm{A}} = 1$$

$$\widehat{\mathrm{A}}^\dagger\psi_n(x) = \sqrt{n+1}\,\psi_{n+1}(x) \qquad \widehat{\mathrm{A}}\,\psi_n(x) = \sqrt{n}\,\psi_{n-1}(x) \qquad \widehat{\mathrm{A}}\,\psi_0(x) = 0$$

$$\widehat{\mathrm{x}} = \frac{a}{\sqrt{2}}\left(\widehat{\mathrm{A}} + \widehat{\mathrm{A}}^\dagger\right) \qquad \widehat{\mathrm{p}}_x = \frac{-\mathrm{i}\hbar}{a\sqrt{2}}\left(\widehat{\mathrm{A}} - \widehat{\mathrm{A}}^\dagger\right)$$

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}A(k)\,\mathrm{e}^{\mathrm{i}(kx-E_kt/\hbar)}\,\mathrm{d}k \qquad A(k) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\Psi(x,0)\,\mathrm{e}^{-\mathrm{i}kx}\,\mathrm{d}x$$

$$\int_{-\infty}^{\infty}|A(k)|^2\,\mathrm{d}k = 1 \qquad \langle p_x\rangle = \int_{-\infty}^{\infty}\hbar k\,|A(k)|^2\,\mathrm{d}k$$

$$j_x(x,t) = -\frac{\mathrm{i}\hbar}{2m}\left(\Psi^*\frac{\partial\Psi}{\partial x} - \Psi\frac{\partial\Psi^*}{\partial x}\right) \qquad T = \frac{4k_1k_2}{(k_1+k_2)^2}$$

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3.1 PT/TEX

Quantum mechanics and its interpretation

$$\langle f|g\rangle = \int_{-\infty}^{\infty} f^*(x)g(x)\,\mathrm{d}x \qquad \langle f|g\rangle = \langle g|f\rangle^*$$

$$\Big\langle f\Big|\sum_i c_i g_i\Big\rangle = \sum_i c_i\langle f|g_i\rangle \qquad \Big\langle \sum_i c_i g_i\Big|f\Big\rangle = \sum_i c_i^*\langle g_i|f\rangle$$

$$\langle f|\widehat{\mathrm{A}}g\rangle = \langle \widehat{\mathrm{A}}f|g\rangle \qquad \langle f|f\rangle\langle g|g\rangle \geq \big|\langle f|g\rangle\big|^2$$

$$\big[\widehat{\mathrm{A}},\widehat{\mathrm{B}}\big] = \widehat{\mathrm{A}}\widehat{\mathrm{B}} - \widehat{\mathrm{B}}\widehat{\mathrm{A}} \qquad \big[\widehat{\mathrm{x}},\widehat{\mathrm{p}}_x\big] = \mathrm{i}\hbar.$$

$$\frac{\mathrm{d}\langle A\rangle}{\mathrm{d}t} = \frac{1}{\mathrm{i}\hbar}\Big\langle[\widehat{\mathrm{A}},\,\widehat{\mathrm{H}}]\Big\rangle \qquad \Delta A\,\Delta B \geq \frac{1}{2}\Big|\Big\langle[\widehat{\mathrm{A}},\,\widehat{\mathrm{B}}]\Big\rangle\Big|$$

$$L_z = xp_y - yp_x \qquad L = I\omega$$

$$E_{\mathrm{rot}} = \frac{L^2}{2I} \qquad \boldsymbol{\mu} = I\mathbf{A} = \gamma\mathbf{L}$$

$$\widehat{\mathrm{L}}_z = -\mathrm{i}\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right] \qquad \widehat{\mathrm{L}}_z = -\mathrm{i}\hbar\frac{\partial}{\partial\phi} \qquad \widehat{\mathrm{L}}^2 = \widehat{\mathrm{L}}_x^2 + \widehat{\mathrm{L}}_y^2 + \widehat{\mathrm{L}}_z^2$$

$$\big[\widehat{\mathrm{L}}_x,\widehat{\mathrm{L}}_y\big] = \mathrm{i}\hbar\widehat{\mathrm{L}}_z \qquad \big[\widehat{\mathrm{L}}_y,\widehat{\mathrm{L}}_z\big] = \mathrm{i}\hbar\widehat{\mathrm{L}}_x \qquad \big[\widehat{\mathrm{L}}_z,\widehat{\mathrm{L}}_x\big] = \mathrm{i}\hbar\widehat{\mathrm{L}}_y \qquad \big[\widehat{\mathrm{L}}^2,\,\widehat{\mathrm{L}}_z\big] = 0$$

$$L^2 = l(l+1)\hbar^2, \qquad l = 0,1,2,\ldots \qquad L_z = m\hbar, \qquad m = 0,\pm1,\ldots,\pm l$$

$$\big[\widehat{\mathrm{S}}_x,\widehat{\mathrm{S}}_y\big] = \mathrm{i}\hbar\,\widehat{\mathrm{S}}_z \qquad \big[\widehat{\mathrm{S}}_y,\widehat{\mathrm{S}}_z\big] = \mathrm{i}\hbar\,\widehat{\mathrm{S}}_x \qquad \big[\widehat{\mathrm{S}}_z,\widehat{\mathrm{S}}_x\big] = \mathrm{i}\hbar\,\widehat{\mathrm{S}}_y \qquad \big[\widehat{\mathrm{S}}^2,\,\widehat{\mathrm{S}}_z\big] = 0$$

$$S^2 = s(s+1)\hbar^2, \qquad s = \tfrac{1}{2} \qquad S_z = m_s\hbar, \qquad m_s = \pm\tfrac{1}{2}$$

$$\boldsymbol{\mu} = \gamma_s\mathbf{S} \qquad \widehat{\mathrm{H}} = -\gamma_s B\widehat{\mathrm{S}}_{\mathbf{n}}$$

$$\widehat{\mathrm{S}}_{\mathbf{n}} = \frac{\hbar}{2}\begin{bmatrix}\cos\theta & \mathrm{e}^{-\mathrm{i}\phi}\sin\theta\\ \mathrm{e}^{\mathrm{i}\phi}\sin\theta & -\cos\theta\end{bmatrix} \qquad |\uparrow_{\mathbf{n}}\rangle = \begin{bmatrix}\cos(\theta/2)\\ \mathrm{e}^{\mathrm{i}\phi}\sin(\theta/2)\end{bmatrix} \qquad |\downarrow_{\mathbf{n}}\rangle = \begin{bmatrix}-\mathrm{e}^{-\mathrm{i}\phi}\sin(\theta/2)\\ \cos(\theta/2)\end{bmatrix}$$

$$\widehat{\mathrm{S}}_x = \frac{\hbar}{2}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} \qquad \widehat{\mathrm{S}}_y = \frac{\hbar}{2}\begin{bmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{bmatrix} \qquad \widehat{\mathrm{S}}_z = \frac{\hbar}{2}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

$$\tfrac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\big) = |0,0\rangle$$

$$\tfrac{1}{\sqrt{2}}\big(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\big) = |1,0\rangle \qquad |\uparrow\uparrow\rangle = |1,1\rangle \qquad |\downarrow\downarrow\rangle = |1,-1\rangle$$

$$C(\theta_1,\theta_2) = P_{++}(\theta_1,\theta_2) + P_{--}(\theta_1,\theta_2) - P_{+-}(\theta_1,\theta_2) - P_{-+}(\theta_1,\theta_2)$$

$$\Sigma = C(\theta_1-\theta_2) + C(\theta_1-\theta_2') + C(\theta_1'-\theta_2) - C(\theta_1'-\theta_2') \qquad |\Sigma| \leq 2$$

Quantum mechanics of matter

$$Y_{lm}(\theta,\phi) = \Theta_{lm}(\theta)\,\mathrm{e}^{\mathrm{i}m\phi} \qquad \widehat{\mathrm{L}}^2 Y_{lm} = l(l+1)\hbar^2\,Y_{lm} \qquad l = 0, 1, 2, \ldots, \qquad m = 0, \pm 1, \ldots, \pm l$$

$$\widehat{\mathrm{L}}_z Y_{lm} = m\hbar\,Y_{lm} \qquad \widehat{\mathrm{L}}^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

$$\text{parity of } Y_{lm} = (-1)^l \qquad \int_0^{2\pi}\int_0^{\pi} Y^*_{l_1,m_1}(\theta,\phi)\,Y_{l_2,m_2}(\theta,\phi)\,\sin\theta\,\mathrm{d}\theta\,\mathrm{d}\phi = \delta_{l_1,l_2}\,\delta_{m_1,m_2}$$

$$\widehat{\mathrm{H}}\psi_n = E_n\psi_n \qquad n = 1, 2, \ldots \qquad \widehat{\mathrm{H}} = -\frac{\hbar^2}{2\mu}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) + \frac{\widehat{\mathrm{L}}^2}{2\mu\,r^2} - \frac{e^2}{4\pi\varepsilon_0\,r}$$

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(r)\,Y_{lm}(\theta,\phi) \qquad R_{nl}(r) = \left(\frac{r}{a_0}\right)^l\left(\text{polynomial in }\frac{r}{a_0}\right)\mathrm{e}^{-r/na_0}$$

$$\langle r^k\rangle = \int_0^\infty r^{k+2}R^2_{nl}(r)\,\mathrm{d}r \qquad \int_0^\infty R^*_{n_1,l}(r)\,R_{n_2,l}(r)\,r^2\,\mathrm{d}r = \delta_{n_1,n_2}$$

$$E_n = -\frac{E_\mathrm{R}}{n^2} \qquad E_\mathrm{R} = \left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\frac{\mu}{2\hbar^2} = \frac{\hbar^2}{2\mu a_0^2} = \frac{1}{2}\,\frac{e^2}{4\pi\varepsilon_0 a_0} \qquad \mu = \frac{m_1 m_2}{m_1 + m_2}$$

$$a_0 = \frac{4\pi\varepsilon_0}{e^2}\frac{\hbar^2}{\mu} \qquad E_{nj} = -\frac{E_\mathrm{R}}{n^2}\left[1 + \frac{\alpha^2}{n}\left(\frac{1}{j+\frac{1}{2}} - \frac{3}{4n}\right)\right] \qquad \alpha = \frac{e^2}{4\pi\varepsilon_0\hbar c}$$

$$E_\mathrm{R}^\text{scaled} = Z^2\frac{\mu}{\mu_\mathrm{H}}E_\mathrm{R} \qquad a_0^\text{scaled} = \frac{1}{Z}\frac{\mu_\mathrm{H}}{\mu}a_0 \qquad j = l \pm \tfrac{1}{2}$$

$$L = |l_1 - l_2|,\ |l_1 - l_2| + 1,\ \ldots,\ l_1 + l_2 - 1,\ l_1 + l_2 \qquad S = |s_1 - s_2|,\ |s_1 - s_2| + 1,\ \ldots,\ s_1 + s_2 - 1,\ s_1 + s_2$$

$$J = |L - S|,\ |L - S| + 1,\ \ldots,\ L + S - 1, L + S \qquad \mathbf{J} = \mathbf{L} + \mathbf{S} \qquad E_\mathrm{gs} \le \min\frac{\langle\phi_\mathrm{t}|\widehat{\mathrm{H}}|\phi_\mathrm{t}\rangle}{\langle\,\phi_\mathrm{t}|\phi_\mathrm{t}\,\rangle}$$

$$\widehat{\mathrm{H}} = \widehat{\mathrm{H}}^{(0)} + \delta\widehat{\mathrm{H}} \qquad \widehat{\mathrm{H}}^{(0)}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \qquad E_n \simeq E_n^{(0)} + \langle\psi_n^{(0)}|\delta\widehat{\mathrm{H}}|\psi_n^{(0)}\rangle$$

$$\Psi(x,t) = \sum_k a_k(t)\,\psi_k(x)\,\mathrm{e}^{-\mathrm{i}E_k t/\hbar} \qquad a_k(t) \simeq \delta_{ki} + \frac{1}{\mathrm{i}\hbar}\int_0^t \mathrm{e}^{\mathrm{i}\omega_{ki}t'}V_{ki}(t')\,\mathrm{d}t' \qquad l_f = l_i \pm 1;\ m_f = m_i \text{ or } m_i \pm 1$$

Mathematics

$z = x + \mathrm{i}y = r\mathrm{e}^{\mathrm{i}\theta}$

$z^* = x - \mathrm{i}y = r\mathrm{e}^{-\mathrm{i}\theta}$

$|z|^2 = zz^* = x^2 + y^2 = r^2$

$\mathrm{Re}(z) = \dfrac{z + z^*}{2}$

$\mathrm{Im}(z) = \dfrac{z - z^*}{2\mathrm{i}}$

$z^n = r^n \mathrm{e}^{\mathrm{i}n\theta}$

$\mathrm{e}^{\mathrm{i}\theta} = \cos\theta + \mathrm{i}\sin\theta$

$\cos\theta = \dfrac{\mathrm{e}^{\mathrm{i}\theta} + \mathrm{e}^{-\mathrm{i}\theta}}{2}$

$\sin\theta = \dfrac{\mathrm{e}^{\mathrm{i}\theta} - \mathrm{e}^{-\mathrm{i}\theta}}{2\mathrm{i}}$

$\mathrm{e}^{\pm\mathrm{i}\pi} = -1$

$\mathrm{e}^{\mathrm{i}\pi/2} = \mathrm{i}$

$\mathrm{e}^{-\mathrm{i}\pi/2} = -\mathrm{i}$

$\mathrm{e}^x \mathrm{e}^y = \mathrm{e}^{x+y}$

$\ln a + \ln b = \ln(ab) \quad (a > 0, b > 0)$

$\mathrm{e}^{\ln a} = \ln(\mathrm{e}^a) = a \quad (a > 0)$

$\cos(\theta \pm \pi) = -\cos\theta$

$\sin(\theta \pm \pi) = -\sin\theta$

$\tan(\theta \pm \pi) = \tan\theta$

$\cos(\theta \pm \pi/2) = \mp\sin\theta$

$\sin(\theta \pm \pi/2) = \pm\cos\theta$

$\tan(\theta \pm \pi/2) = -\cot\theta$

$\cos^2\theta + \sin^2\theta = 1$

$\dfrac{1}{1+x} = 1 - x + x^2 - \ldots$

$\dfrac{1}{1-x} = 1 + x + x^2 + \ldots$

$e^x = 1 + x + \dfrac{x^2}{2!} + \dfrac{x^3}{3!} + \ldots$

$\cos x = 1 - \dfrac{x^2}{2!} + \dfrac{x^4}{4!} - \ldots$

$\sin x = x - \dfrac{x^3}{3!} + \dfrac{x^5}{5!} - \ldots$

$\cos(A \pm B) = \cos A\cos B \mp \sin A\sin B$

$\sin(A \pm B) = \sin A\cos B \pm \cos A\sin B$

$\cos A\cos B = \frac{1}{2}\big(\cos(A-B) + \cos(A+B)\big)$

$\sin A\sin B = \frac{1}{2}\big(\cos(A-B) - \cos(A+B)\big)$

$\mathrm{d}f/\mathrm{d}x$	$f(x)$	$\int f(x)\,\mathrm{d}x$
nx^{n-1}	x^n	$\frac{1}{n+1}x^{n+1} + C \quad (n \neq -1)$
$-1/x^2$	$1/x$	$\ln x + C$
$a\cos(ax)$	$\sin(ax)$	$-\frac{1}{a}\cos(ax) + C$
$-a\sin(ax)$	$\cos(ax)$	$\frac{1}{a}\sin(ax) + C$
$a\exp(ax)$	$\exp(ax)$	$\frac{1}{a}\exp(ax) + C$
$1/x$	$\ln(ax)$	$x\,\ln(ax) - x + C$

Physical constants

Planck's constant	h	$6.63 \times 10^{-34}\,\mathrm{J\,s}$	Planck's constant/2π	$\hbar$	$1.06 \times 10^{-34}\,\mathrm{J\,s}$
vacuum speed of light	c	$3.00 \times 10^{8}\,\mathrm{m\,s^{-1}}$	Coulomb law constant	$\frac{1}{4\pi\varepsilon_0}$	$8.99 \times 10^{9}\,\mathrm{m\,F^{-1}}$
permittivity of free space	ε_0	$8.85 \times 10^{-12}\,\mathrm{F\,m^{-1}}$	permeability of free space	μ_0	$4\pi \times 10^{-7}\,\mathrm{H\,m^{-1}}$
Boltzmann's constant	k	$1.38 \times 10^{-23}\,\mathrm{J\,K^{-1}}$	Avogadro's constant	N_m	$6.02 \times 10^{23}\,\mathrm{mol^{-1}}$
electron charge	$-e$	$-1.60 \times 10^{-19}\,\mathrm{C}$	proton charge	e	$1.60 \times 10^{-19}\,\mathrm{C}$
electron mass	m_e	$9.11 \times 10^{-31}\,\mathrm{kg}$	proton mass	m_p	$1.67 \times 10^{-27}\,\mathrm{kg}$
atomic mass unit	u	$1.66 \times 10^{-27}\,\mathrm{kg}$	neutron mass	m_n	$1.67 \times 10^{-27}\,\mathrm{kg}$
Bohr radius	a_0	$5.29 \times 10^{-11}\,\mathrm{m}$	fine structure constant	α	$1/137$
electronvolt	eV	$1.60 \times 10^{-19}\,\mathrm{J}$	Rydberg energy	E_R	$13.6\,\mathrm{eV}$